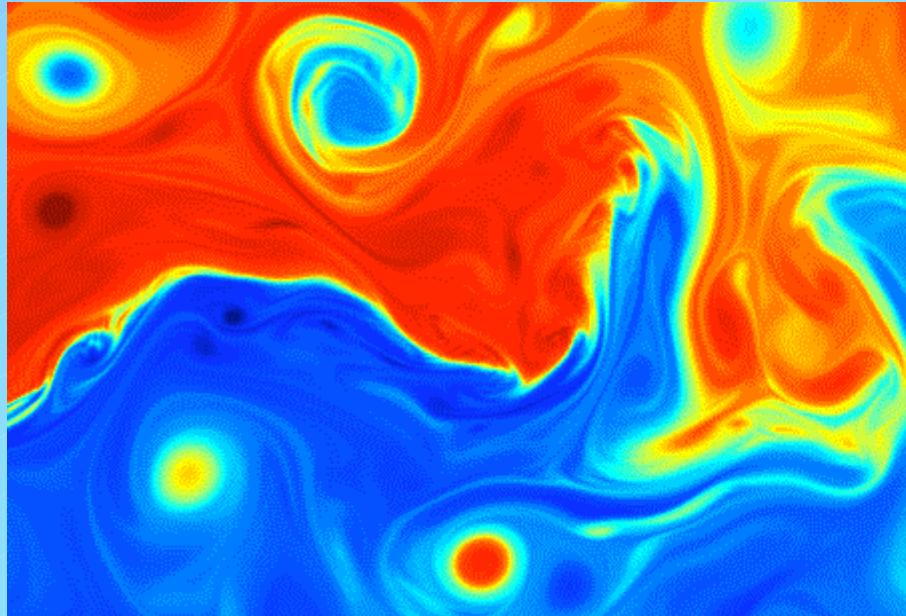


Parallelization of a Spectral Fluid Model

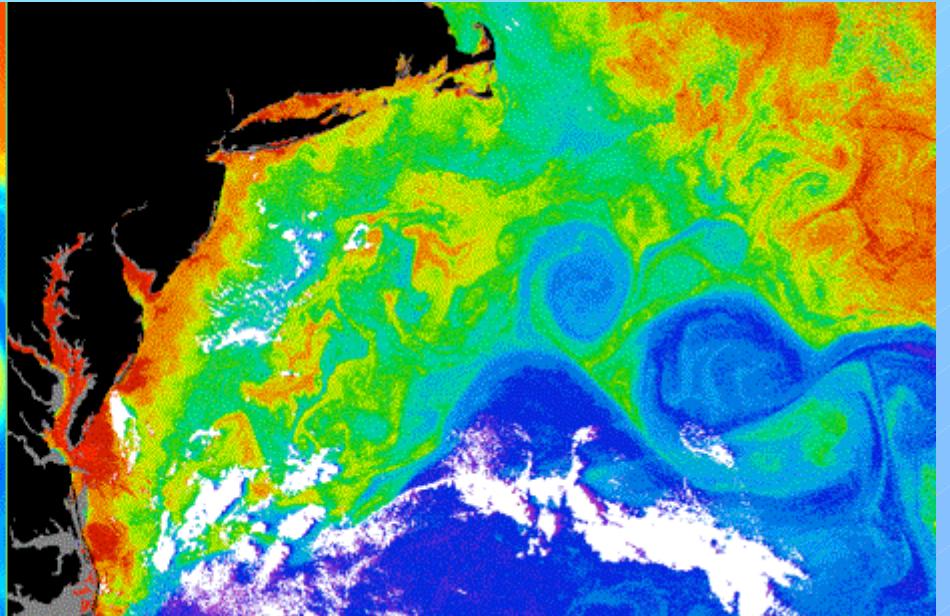
Mark Petersen

NASA High Performance Computing Summer School, July 2003

Quasi-Geostrophic model



Actual sea surface temperature



Funded by Vigre and NSF OCE 0137347

The Governing Equations

- **Conservation of Momentum:** Navier-Stokes Equation

$$\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho_o} \nabla p + 2\Omega \mathbf{\hat{z}} \times \mathbf{u} + b\hat{z} + \kappa^2 \mathbf{u}$$

advection pressure Coriolis buoyancy diffusion
(wind) gradient force

- **Conservation of Energy:** Buoyancy anomaly

$$\partial_t b + \mathbf{u} \cdot \nabla b = N^2(z)w + k\nu^2 b$$

advection stratification diffusion

- **Conservation of Mass** for incompressible fluid

$$\nabla \cdot \mathbf{u} = 0$$

To Simplify the Primitive Equations:

Assume Coriolis forces are stronger than advection (winds)

Rossby Number $R_o = \frac{U}{\square L} = \frac{U^2/L}{\square U} = \frac{\text{advection}}{\text{Coriolis}} \ll 1$

Now expand all variables about this small parameter

$$\mathbf{u} = \mathbf{u}_0 + R_o \mathbf{u}_1 + R_o^2 \mathbf{u}_2 \dots$$

$$p = p_0 + R_o p_1 + R_o^2 p_2 \dots$$

Vary the aspect ratio to derive a suite of regimes:

QG



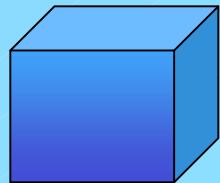
$$H/L \ll 1$$

$$R_o \ll 1$$

$$Fr \ll 1$$

Charney 1948

Intermediate



$$H/L = O(1)$$

$$R_o \ll 1$$

$$Fr \ll 1$$

*Embidi & Majda
1998*

Convection



$$H/L \gg 1$$

$$R_o \ll 1$$

$$Fr = O(1)$$

*Julien, Knobloch,
Werne 1998*

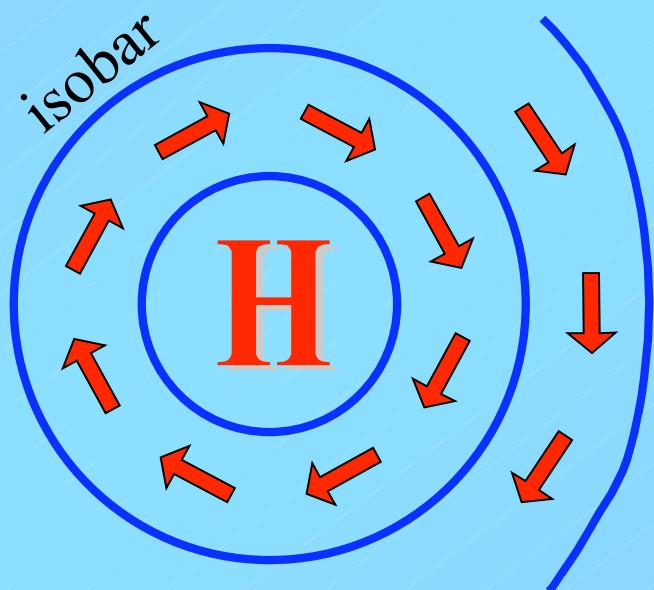
QG Regime: Leading Order

Geostrophic Flow

$$\square_3 \square \mathbf{u}_0 = \square \square \square p_0$$

Coriolis
force

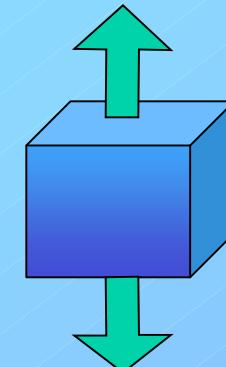
pressure
gradient



Hydrostatic Balance

$$\partial_z p_0 = \square b_0 \hat{z}$$

pressure
gradient



QG Regime: Higher Order

Quasi-Geostrophic Momentum

$$(\partial_t + \mathbf{u}_0 \cdot \nabla) \mathbf{u}_0 = -\frac{1}{\rho g} \nabla p_1 - \frac{1}{\text{Re } R_o^2} \partial_z^2 \mathbf{u}_0$$

$\mathbf{u}_0 = (u_0, v_0, 0)$ is the geostrophic velocity

$\mathbf{u}_1 = (u_1, v_1, 0)$ is the ageostrophic velocity

Buoyancy equations tell us

$$w_0 = 0$$

$$w_1 = 0$$



QG Potential Vorticity Equation

Curl of Navier-Stokes, substitute w_2 from energy equation:

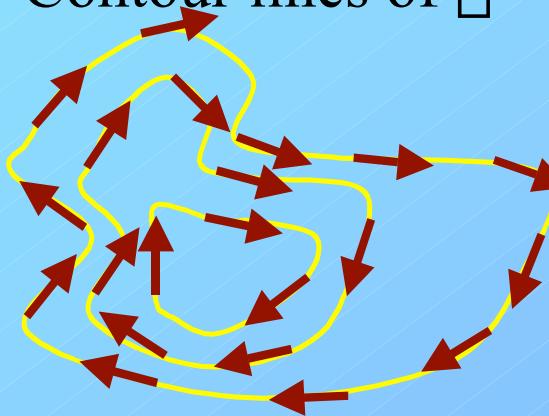
$$D_t \left(\frac{\partial^2 \psi}{\partial z^2} + \frac{\partial^2 \psi}{\partial z^2} \partial_z \frac{\partial_z \psi}{S(z)} \right) = \frac{1}{\text{Re } R_o^2} \partial_{zz} \left(\frac{\partial^2 \psi}{\partial z^2} \right) + \frac{\partial^2 \psi}{\partial z^2} \partial_z \frac{\partial_{zzz} \psi}{S(z)}$$

vorticity stretching vorticity buoyancy
 dissipation forcing/dissipation

$$D_t = \partial_t + u_0 \partial_x + v_0 \partial_y$$

ψ is stream function
 S is stratification

Contour lines of ψ



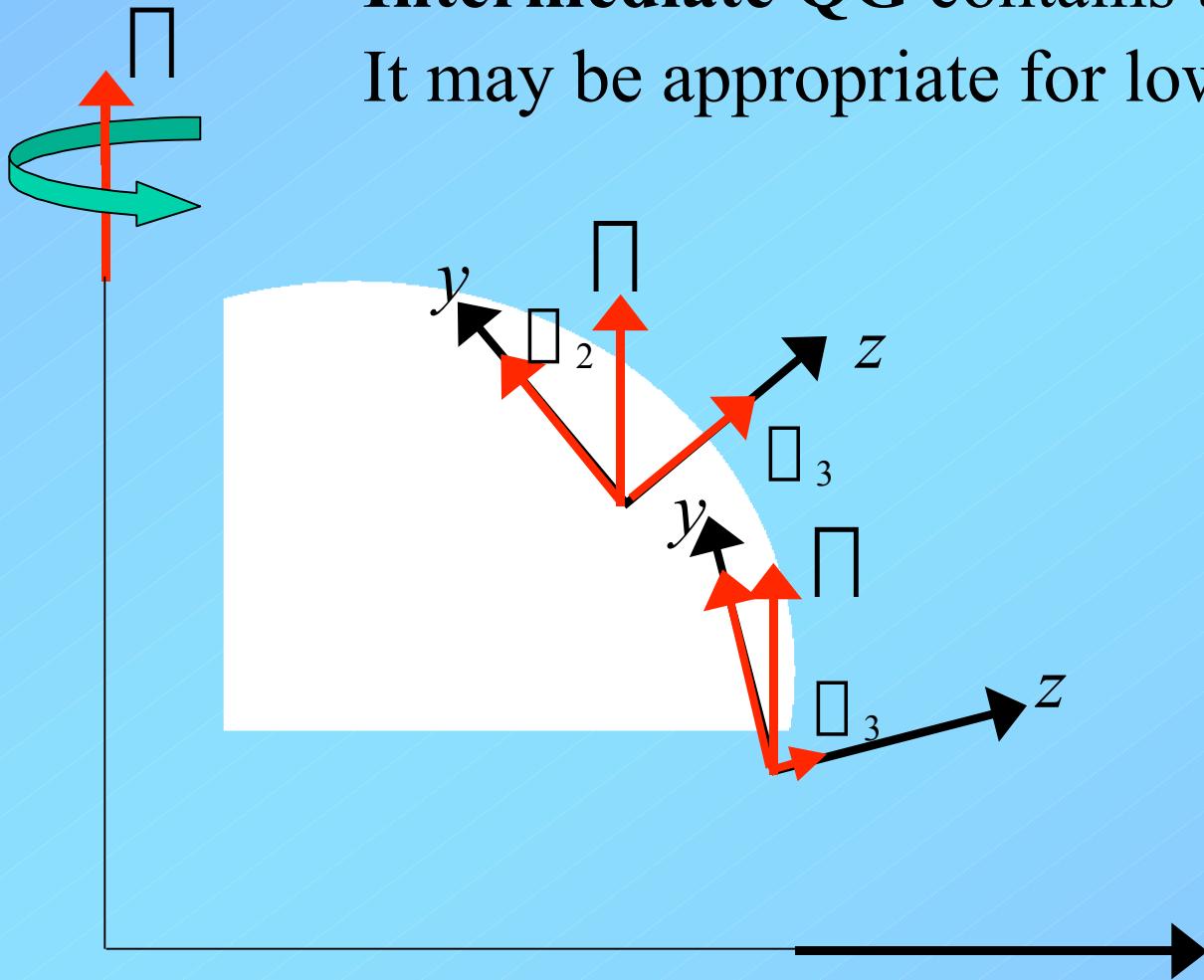
$$u = \psi \partial_y \psi, \quad v = \partial_x \psi$$

QG contains only the \bar{U}_3 component.

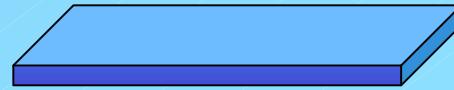
It is valid at midlatitudes but not near the equator.

Intermediate QG contains the full \bar{U} vector.

It may be appropriate for low latitude dynamics.

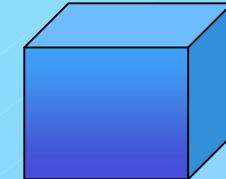


QG Regime



$$D_t \left[\frac{\partial}{\partial z} \left(\frac{\partial_z \bar{u}}{S(z)} \right) \right] + \bar{u}_3^2 \partial_z \frac{\partial_z \bar{u}}{S(z)} = \frac{1}{\text{Re} R_o^2} \partial_{zz} \bar{u} \bar{u}^2 + \frac{\bar{u}_3^2}{Pe R_o^2} \partial_z \frac{\partial_{zzz} \bar{u}}{S(z)}$$

Intermediate Regime



$$D_t \left[\frac{\partial}{\partial z} \left(\frac{\partial_z \bar{u}}{S(z)} \right) \right] + (\bar{u} \cdot \bar{u}) \frac{(\bar{u} \cdot \bar{u}) \bar{u}}{S(z)} = \frac{1}{\text{Re}} \bar{u}^2 \bar{u}^2 + \frac{(\bar{u} \cdot \bar{u}) \bar{u}^2 (\bar{u} \cdot \bar{u}) \bar{u}}{Pe S(z)}$$

IQG Potential Vorticity Equation

$$\begin{aligned}\partial_t q + J(\psi, q) &= \frac{1}{\text{Re}} \nabla^2 \psi \cdot \nabla^2 \psi + \frac{1}{SPe} (\nabla \cdot \nabla)^2 \psi^2 \\ q &= \nabla^2 \psi + \frac{1}{S} (\nabla \cdot \nabla)^2 \psi\end{aligned}$$

$$\begin{aligned}\partial_t q + J(\psi, q) &= L\psi \\ q &= M\psi\end{aligned}$$

ψ streamfunction,

q potential vorticity

L, M linear diffusive operators

J nonlinear advection term

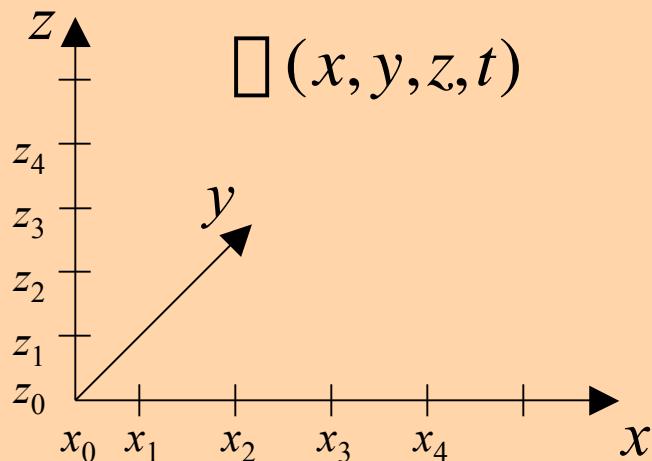
$$J = \partial_x \psi \partial_y q - \partial_y \psi \partial_x q$$

Numerical Method: Pseudo-Spectral

$$\boxed{\partial_t q + J(\square, q) = L\square}$$
$$q = M\square$$

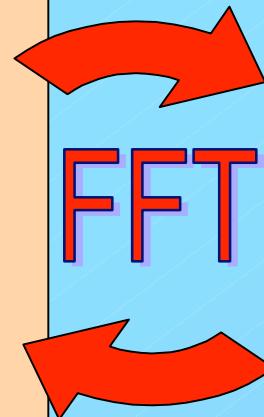
Time stepping: Third order Runge-Kutta
Domain: 3D periodic boundaries
Basis Functions: Fourier Series

Physical Space

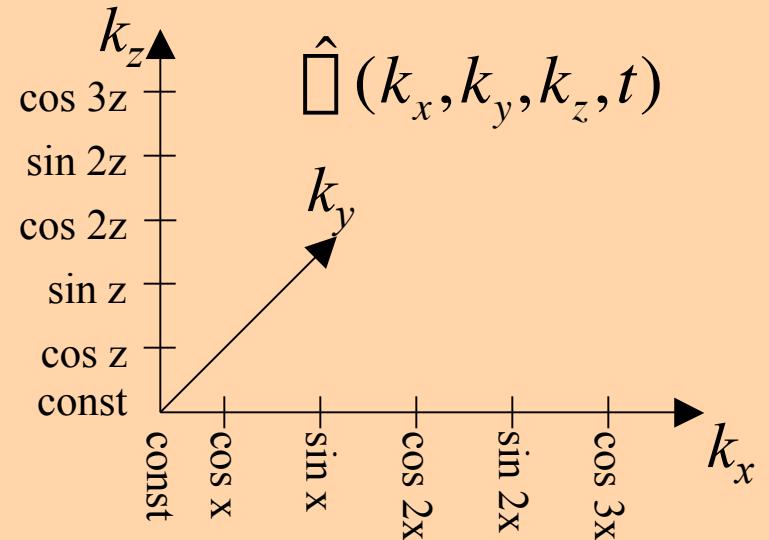


Nonlinear terms easy

$$J = \partial_x \square \partial_y q \square \partial_y \square \partial_x q$$



Fourier Space



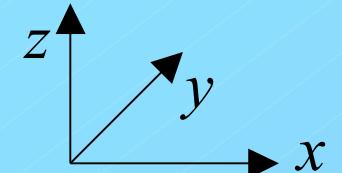
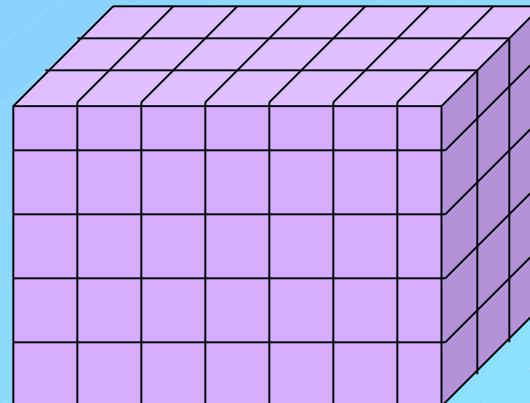
Derivatives are cheap!

$$\square^2 \hat{\square} = \square(k_x^2 + k_y^2 + k_z^2) \hat{\square}$$

How we see an array:

$$A(i, j, k)$$

$A(1,1,5)$
 $A(1,1,4)$
 $A(1,1,3)$
 $A(1,1,2)$
 $A(1,1,1)$



How FORTRAN sees an array:

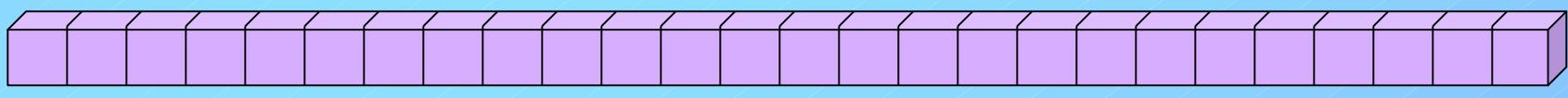
$A(1,1,1)$
 $A(2,1,1)$
 $A(3,1,1)$
 $A(4,1,1)$
⋮

$A(n,1,1)$
 $A(1,2,1)$
 $A(2,2,1)$
 $A(3,2,1)$
 $A(4,2,1)$
⋮

$A(n,2,1)$
 $A(1,3,1)$
 $A(2,3,1)$
 $A(3,3,1)$
 $A(4,3,1)$
⋮

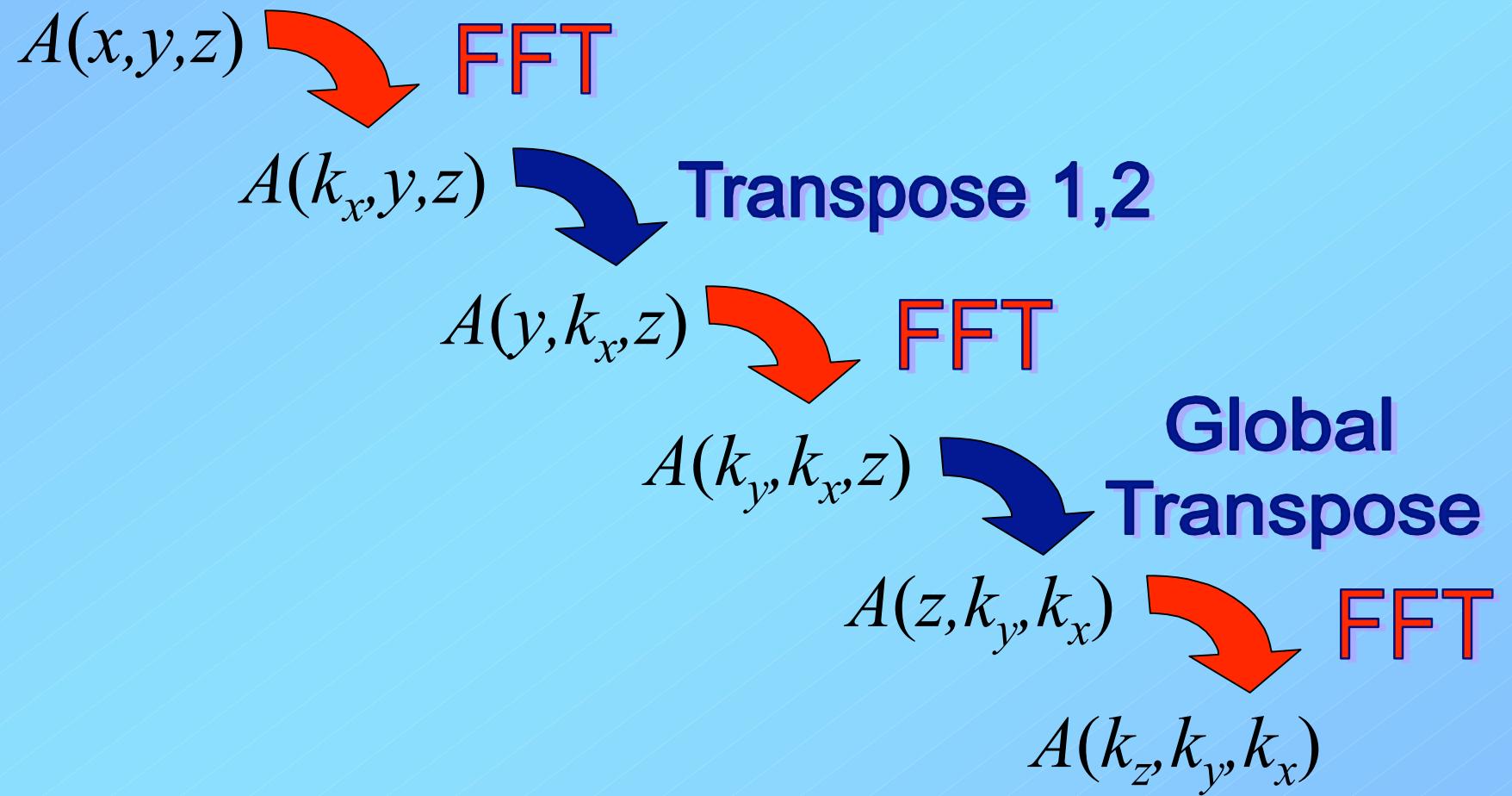
$A(1,1,1)$
 $A(2,1,1)$
 $A(3,1,1)$
 $A(4,1,1)$
 $A(5,1,1)$
 $A(6,1,1)$
⋮

⋮ ⋮ ⋮ ⋮ ⋮
 $A(n,n,1)$
 $A(1,1,2)$
 $A(2,1,2)$
 $A(3,1,2)$
 $A(4,1,2)$
⋮



Each one dimensional FFT must be done on the first index

FFT in Three Dimensions



Implementation of Global Transpose

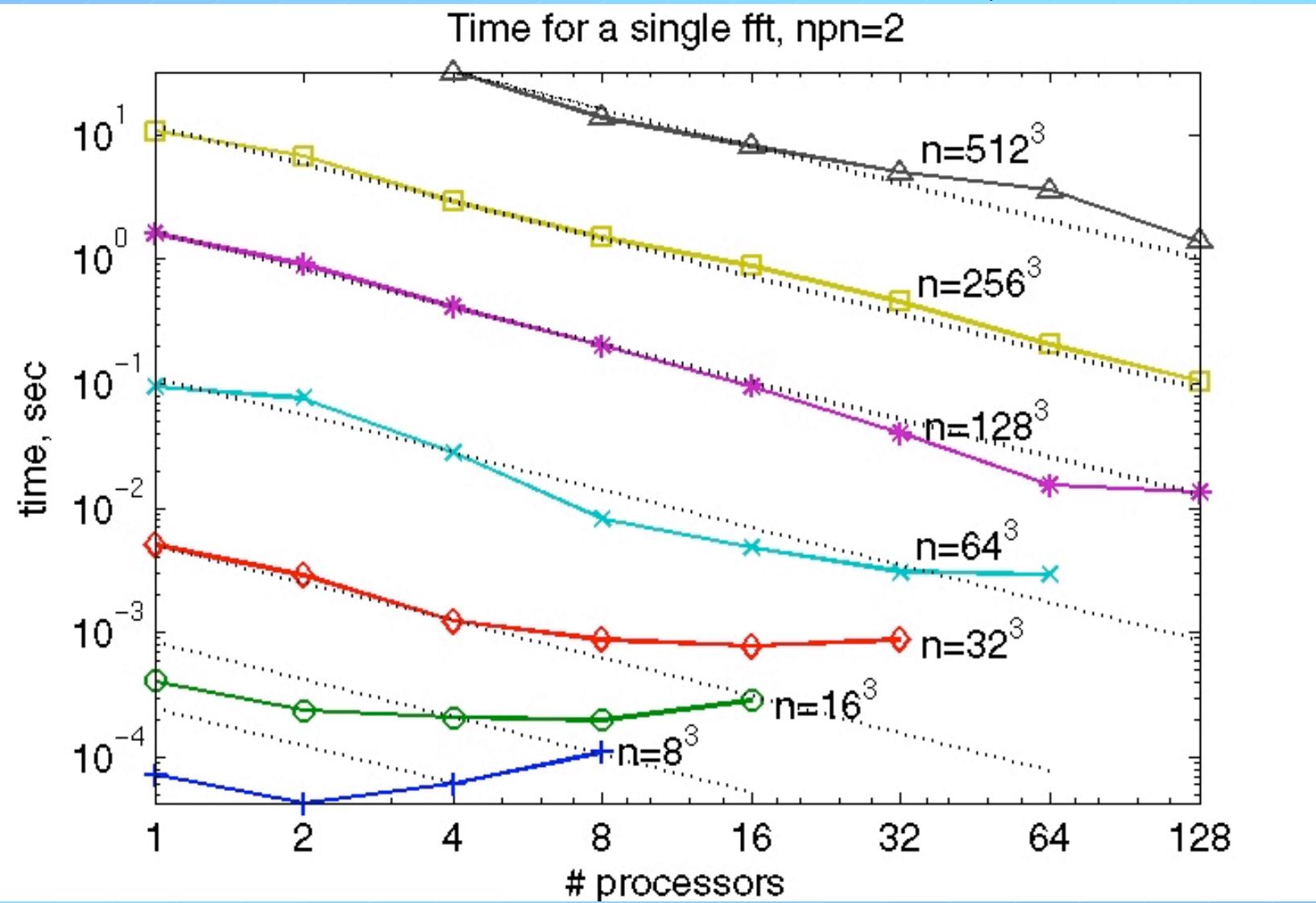
owned by:	P1	P2	P3	P4		
matrix A	1,1 1,2	1,3 1,4	1,5 1,6	1,7 1,8		} send to P1
	2,1 2,2	2,3 2,4	2,5 2,6	2,7 2,8		} send to P2
	3,1 3,2	3,3 3,4	3,5 3,6	3,7 3,8		} send to P3
	4,1 4,2	4,3 4,4	4,5 4,6	4,7 4,8		} send to P4
	5,1 5,2	5,3 5,4	5,5 5,6	5,7 5,8		
	6,1 6,2	6,3 6,4	6,5 6,6	6,7 6,8		
	7,1 7,2	7,3 7,4	7,5 7,6	7,7 7,8		
	8,1 8,2	8,3 8,4	8,5 8,6	8,7 8,8		

Three step process:

1. Local transpose
2. Send and receive appropriate parts of your matrix
3. Rearrange local matrix

Timing Results

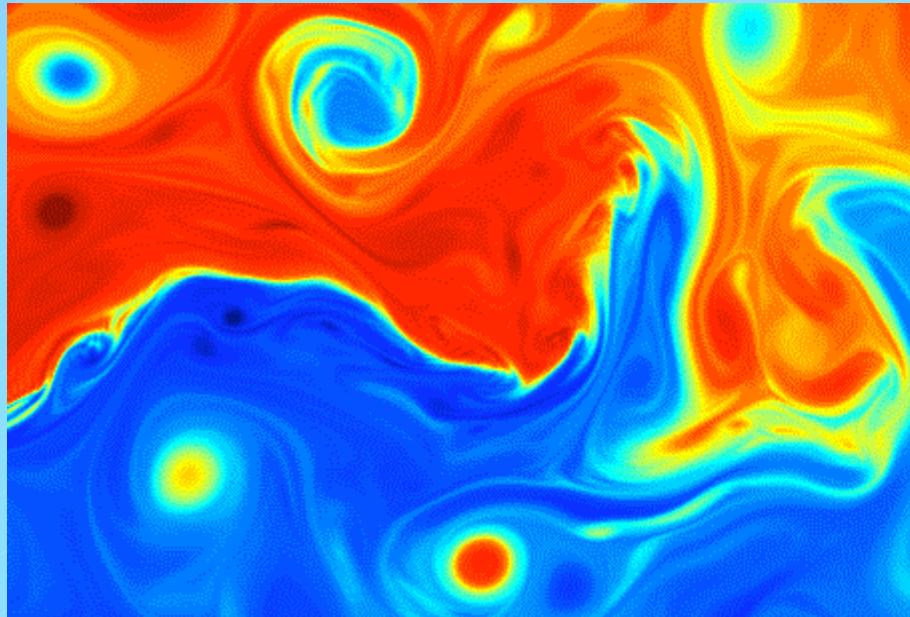
Machine: 64 node, each with:
Dual 2.4 GHz Intel P4 Xeon
512 KB L2 Cache, 2 GB RAM



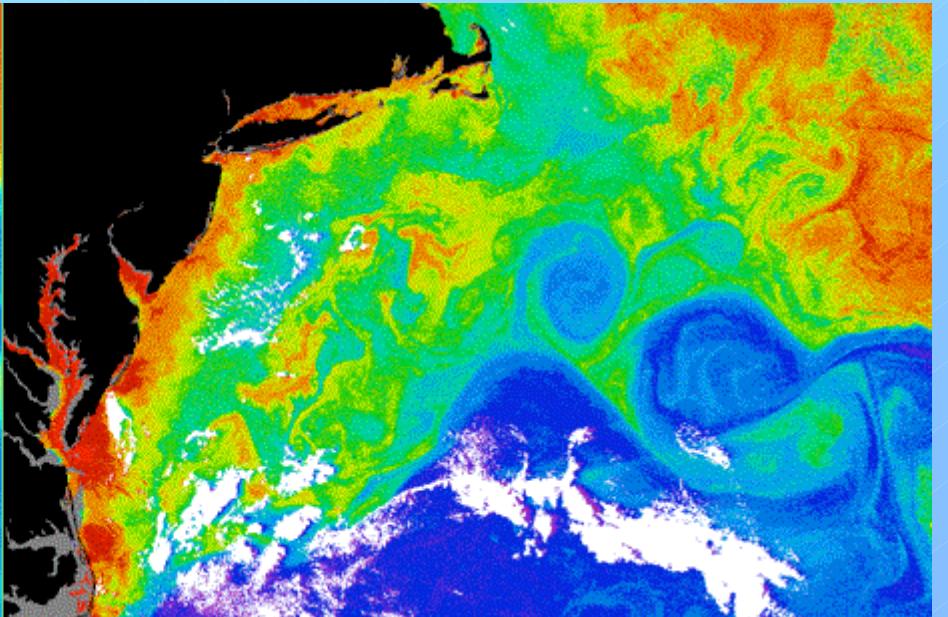
Future Plans

- Implement parallel FFT in the full Quasi-Geostrophic code.
- Observe spectral distribution of energy with time.
- Run comparisons of standard and intermediate QG

Quasi-Geostrophic model



Actual sea surface temperature



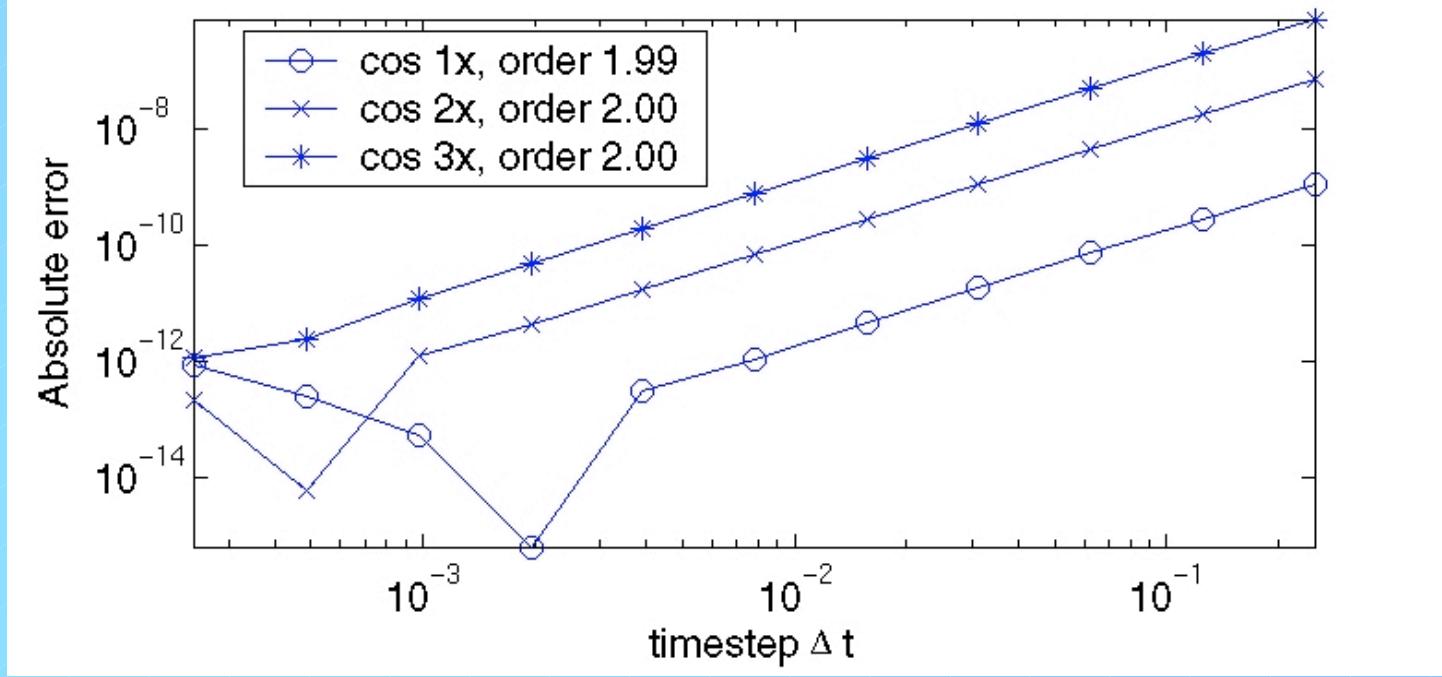
Model Validation, Linear Case

If $\square(x,t)$ only, the IQG equation reduces to

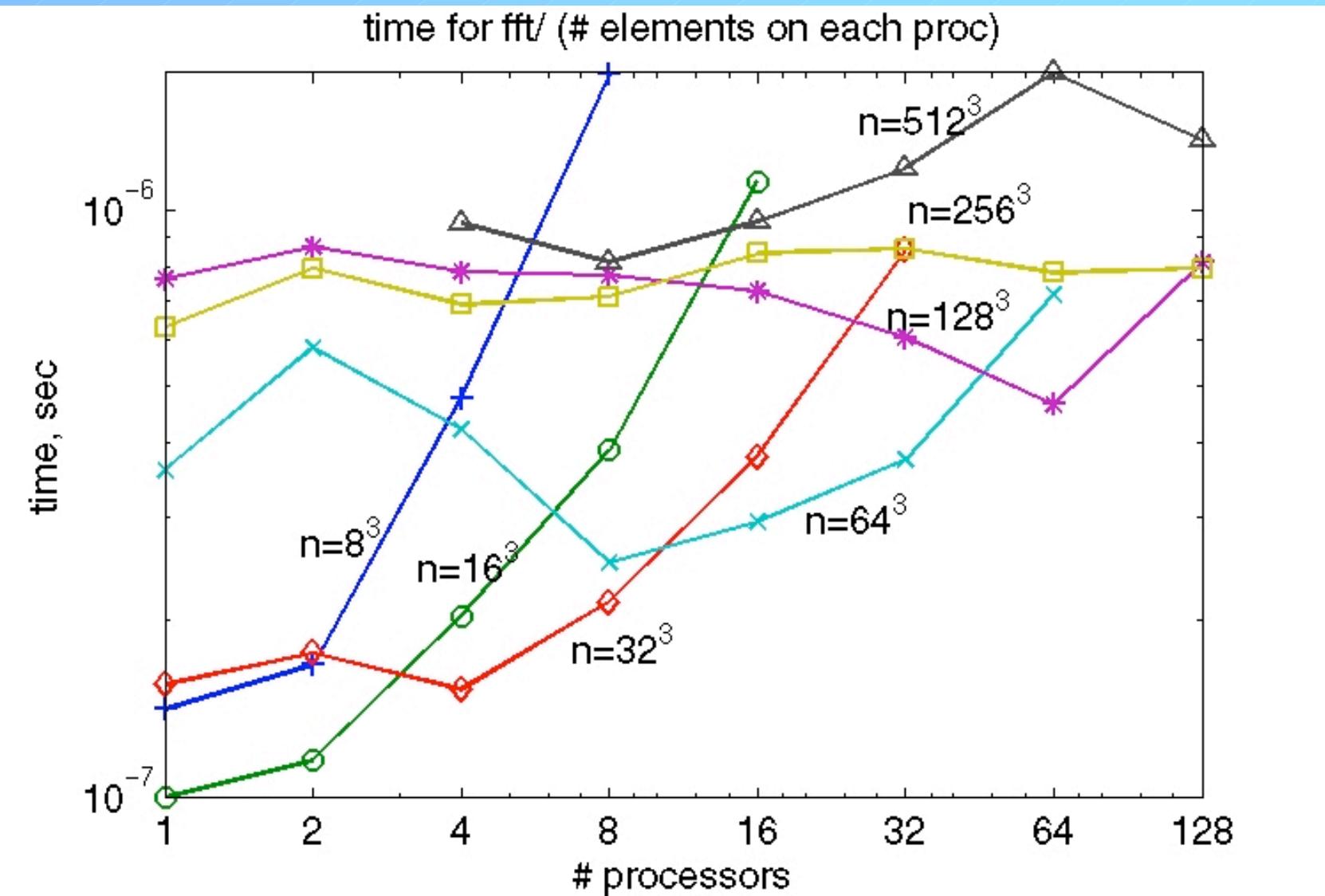
$$\partial_t \partial_x^2 \square = \frac{1}{\text{Re}} \partial_x^4 \square$$

This is the heat equation in $\partial_x^2 \square$ with solution

$$\square(x,t) = \square(x,0)e^{\square t}, \quad \square = \square k_z^2 / \text{Re}$$



Timing Results



Memory Requirements

